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RENORMALIZED LANDAU LEVELS AND PARTICLE-HOLE SYMMETRY IN GRAPHENE

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In this preceedings paper we report on a calculation of graphene's Landau levels in a magnetic field. Our calculations are based on a self-consistent Hartree-Fock approximation for graphene's massless-Dirac continuum model. We find that because of graphene's chiral band structure interactions not only shift Landau-level energies, as in a non-relativistic electron gas, but also alter Landau level wavefunctions. We comment on the subtle continuum model regularization procedure necessary to correctly maintain the lattice-model's particle hole symmetry properties.

Keywords: Graphene; Landau levels; Particle-hole symmetry.

1. Introduction

Graphene, a one-atom-thick two-dimensional crystal of carbon atoms arranged in a honeycomb lattice, is a gapless semiconductor with an unusual massless Dirac-fermion band structure that has long attracted theoretical interest [1,2]. The low-energy properties of graphene are characterized by quasiparticle dispersion [3] linear in momentum and by vanishing density-of-states at the neutral system Fermi energy. The band eigenstates can be considiered as sublattice-pseudospin spinors and have

a chiral property which qualitatively alters the way in which electron-electron inter-actions influence electronic properties. In particular electron-electron interactions lead to a logarithimic enhancement of the Fermi velocity in doped and undoped graphene related to a lack of screening at the Dirac point [4,5,6].

In the presence of a magnetic field, graphene's electronic structure also changes in a nontrivial way when compared to the non-relativistic two dimensional electron gas (2DEG) case, leading to the so-called half-quantized Hall effect [8,7] in which the plateau values of the Hall conductivity are given by $\sigma_{xy} = 4(n + 1/2)(e^2/h)$. Plateau conductivity values are separated by $4e^2/h$ because of the fourfold degeneracy due to valley and spin. In this paper we analyze the effect of electron-electron interactions on graphene's LL spectrum. We show that because of the chiral nature of graphene's band structure, interactions not-only shift Landau level energies but also alter Landau-level wavefunctions.

2. Self Consistent Hartree-Fock Approximation

In this section we use the self-consistent Hartree-Fock approximation (SCHFA) to study the effect of electron-electron interactions on the LL spectium of graphene within the massless Dirac-fermion(MDF) model. The low-energy properties of graphene can be adequately described by a MDF model:

$$\mathcal{H}_{\vec{p}} = v\vec{\sigma} \cdot p \qquad (1)$$

where σ^i's are Pauli matrices acting on graphene's psuedospin degrees of freedom, $\vec{p}$ is a two dimensional vector measured from the Dirac points. (As we will discuss later this model requires especially subtle ultraviolet regularizations in order to yield physically correct predictions.) In the presence of a unifrom magnetic field $\vec{B} = B\hat{z}$ applied in a direction perpendicular to the plane of the graphene sheet 1 is modified by $\vec{p} \to \vec{\pi} = \vec{p} - (e/c)\vec{A}$ where $\vec{A}$ is the vector potential with $\vec{B} = \vec{\nabla} \times \vec{A}$. Defining the usual raising and lowering LL operators $a^\dagger$ and a, with $a^\dagger = (l_B/\sqrt{2}\hbar)\pi$, where $l_B = (\hbar c/eB)^{1/2} = 25.66/\sqrt{(B[\text{T}])}$nm is the magnetic length, we can identify a zero-energy eigenstate given by $a\phi_0 = 0$ and finite-energy chiral eigenatates n and $\bar{n} = -n$ with eigenenergies $\varepsilon_n = sgn(n)\sqrt{\frac{2\hbar v^2 eB|n|}{c}}$. In the Landau gauge $\vec{A} = (0, Bx, 0)$, the corresponding eigenvectors are

$$|\psi_{n\neq0,X}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -isgn(n)\phi_{|n|-1,X} \\ \phi_{|n|,X} \end{pmatrix}, \qquad |\psi_{n=0,X}\rangle = \begin{pmatrix} 0 \\ \phi_{0,X} \end{pmatrix}, \qquad (2)$$

where $\phi_{n,X}$ is a Landau-gauge eigenstate of a non-relatvistic electron gas and X denotes the guiding center degree of freedom within a LL. Projecting the interacting Hamiltonian onto the LL basis gives:

$$\mathcal{H}_{e-e} = \frac{1}{2}\sum_{\vec{q}} v_q : \hat{\rho}(-\vec{q})\hat{\rho}(\vec{q}) :, \qquad (3)$$

where $v_q = 2\pi e^2/\epsilon |q|$ is the two-dimensional Fourier transform of the Coulomb interaction and

$$\hat{\rho}(-\vec{q}) = \sum_{nXn'X'} c^\dagger_{nX\tau s} c_{n'X'\tau's'} \delta(q_y + X - X') e^{iq_x(X' - \frac{q_y}{2})} . F^R_{n,n'}(\vec{q}), \qquad (4)$$

In Eq.(4) $c^\dagger_{nX\tau s}/c_{nX\tau s}$ are creation/annihilation operator for particles in LL n at guiding center X for valley τ and spin s. For notational simplicity we have assumed $l_B = 1$; we will however restore these length units in the final results. $F^R_{n,n'}(\vec{q})$ is referred to as graphene's relativistic form factor and captures the orbital and sublattice pseudospin character of the LL orbitals [9] ($n \neq 0$ and $n' \neq 0$):

$$F^R_{n,n'}(\vec{q}) = \frac{1}{2} \big[F_{|n|,|n'|}(\vec{q}) + sgn(nn') F_{|n|-1,|n'|-1}(\vec{q}) \big], \qquad (5)$$

$F_{|n|,|n'|}(\vec{q})$ is the well known form factor for an ordinary 2DEG [10] in the presence of a perpendicular magnetic field:

$$F_{n,n'}(\vec{q}) = \begin{cases} \sqrt{\frac{n'!}{n!}} \big[i \frac{q_x - iq_y}{\sqrt{2}} \big]^{n-n'} L^{n-n'}_{n'}(\frac{q^2}{2}) e^{-q^2/4} & n \geq n' \\ \sqrt{\frac{n!}{n'!}} \big[i \frac{q_x + iq_y}{\sqrt{2}} \big]^{n'-n} L^{n'-n}_n(\frac{q^2}{2}) e^{-q^2/4} & n' > n, \end{cases} \qquad (6)$$

and the form factor for the lowest LL is just $F^R_{00}(q) = F(q) = e^{-q^2/4}$. Finally

$$F^R_{0,n}(\vec{q}) = \frac{1}{\sqrt{2}} F_{0,n}(\vec{q}) = \sqrt{\frac{1}{2n!}} \big[i \frac{q_x - iq_y}{\sqrt{2}} \big]^n L^n(\frac{q^2}{2}) e^{-q^2/4} \qquad (7)$$

Here $L^{n-n'}_{n'}$ are the associated Laguerre polynomials.

In the Hartree-Fock approximation the effective single-particle Hamiltonian depends on the density matrix. In the case of Landau-level systems, the density-matrix is usefully parameterized as follows:

$$\Delta^{n,n'}_{\tau,\tau',s,s'}(\vec{q}) = \frac{1}{N_\phi} \sum_{X,X'} \langle c^\dagger_{n',X',\tau',s'} c_{n,X,\tau,s} \rangle \delta(q_y + X' - X) . \exp^{-iq_x X} \qquad (8)$$

The Hartree-Fock theory Hamiltonian is expressed in terms of Δ as follows: [a]

$$\langle n, X, \tau, s | \mathcal{H}_{e-e} | n', X', \tau', s' \rangle = \sum_{n_1,n_2} \sum_q \Big[\frac{1}{2\pi l_B^2} V_{n,n',n_2,n_1}(\vec{q}) \Delta^{n_2,n_1}_{\tau",\tau",s",s"}(\vec{q}) \delta^{ss'}_{\tau\tau'} \qquad (9)$$

$$- \frac{1}{L^2} \sum_p V_{n_2,n',n,n_1}(\vec{p}) \Delta^{n_2,n_1}_{\tau,\tau',s,s'}(\vec{q}) \exp^{i(\vec{p} \times \vec{q}) l_B^2 \cdot \hat{z}} \Big] \exp^{iq_x X'} \delta(q_y l_B^2 + X - X')$$

here we restore l_B and define

$$V_{n_1,n_2,n_3,n_4}(\vec{q}) = v_q F^R_{n_1,n_4}(\vec{q}) F^R_{n_2,n_3}(-\vec{q}) \qquad (10)$$

For the purposes of this paper we assume that the translational invariance is not broken. In this case Δ is non-zero only for $\vec{q} = 0$. It follows that

$$\Delta^{n_1,n_2}_{\tau\tau'ss'}(\vec{q}) = \Delta^{n_1,n_2}_{\tau\tau'ss'}(0) \delta_{\vec{q}=0} \delta(|n_1| - |n_2|). \qquad (11)$$

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[a]The details of this calculation are similar to the one in Ref. 10.

The δ function which sets mixing between states with different values of $|n|$ can be seen to follow from spatial isotropy in the continuum model. Because both positive and negative values of n occur in graphene this restriction does not forbid mixing of states with positive and negative n by interactions. The fact that Landau-level wavefunctions are altered by interactions in graphene is the main difference between relativistic and non-relativistic cases.

Assuming no broken translational symmetry, the first term in (9) is just the constant Hartree (electrostatic) potential which can be absorbed in the zero of energy. Dropping this term yields

$$\langle n, X, \tau, s | \mathcal{H} | n', X', \tau', s' \rangle = - \sum_{|n_1| = |n_2|} \frac{1}{L^2} \sum_{\vec{q}} v_q F^R_{n_2, n'}(\vec{q}) F^R_{n, n_1}(-\vec{q}) \Delta^{n_1, n_2}_{\tau \tau' s s'}(0) \delta(X - X')$$
(12)

The mixing between n and $\bar{n}$ LL is due to the fact that the self-energy is not diagonal in the pseudospin as can be seen by examining spatial isotropy consequences more closely. Isotropy is encoded in the form factors in the above equation:

$$F^R_{m, n'}(\vec{q}) F^R_{n, m}(-\vec{q}) = F^R_{m, n'}(\vec{q}) \bar{F}^R_{m, n}(\vec{q}) \sim \exp^{-i\varphi(|n'| - |n|)}$$
(13)

yielding an angular integral that is proportional to $\delta(|n'| - |n|)$ not $\delta(n' - n)$. The other delta function gives $X = X'$. Assuming no spin or valley broken symmetries we can also assume that different valleys can be considered independently. This yields (suppressing the spin and valley indices):

$$\langle n | \mathcal{H}_{e-e} | n' \rangle = - \sum_{|n_1| = |n_2|} \frac{1}{L^2} \sum_{\vec{q}} v_q F^R_{n_2, n'}(\vec{q}) F^R_{n, n_1}(-\vec{q}) \Delta^{n_1, n_2}.$$
(14)

Notice that this matrix element is non-zero only if $|n| = |n'|$.

To compute the matrix elements we have to employ a LL index cutoff reminisent of the high-energy cutoff used in for MDF description of graphene at zero magnetic field. This ultraviolet cutoff plays a role because of the unbounded negative energy sea of the massless Dirac model. Following the procedure used at zero magnetic field, we choose a LL cutoff, a maximum value for $|n|$, M based on the physically natural cutoff of momentum at an inverse lattice constant scale, $k_c \sim 1/a$, and on the semi-classical relationship between momentum and Landau-level index. This yields

$$\hbar v_F k_c = \sqrt{2} \frac{\hbar v_F}{l_B} \sqrt{M}.$$
(15)

Using $k_c \sim 1/a$ where $a = 0.246nm$ is graphene honeycomb lattice constant we get a magnetic field dependent cutoff

$$M \sim \frac{5000}{B[T]}$$
(16)

where B is the magnitude of the magnetic field. We can write the mean field Hartree-Fock hamiltoninan in the $(n, \bar{n})$-sector as a two level system:

$$\mathcal{H}_{MF} = \mathcal{E} + \vec{\mathcal{B}} \cdot \vec{\sigma}$$
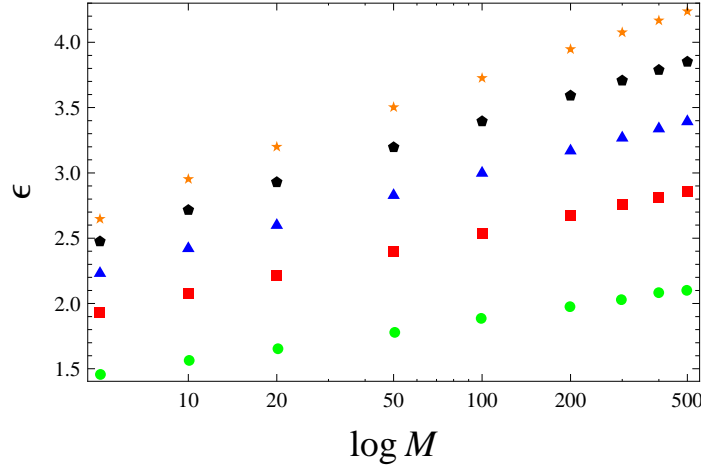(17)

Fig. 1. Hartree-Fock eigenvalues for a neutral graphene sheet in the units $\sqrt{2}\hbar v/l_B$ with $\alpha_{gr} = 2.2$. In this calculation the energy of the $n = 0$ Landau level is chosen as the zero of energy so that all $n \neq 0$ eigenstatesoccur in particle-hole symmetric positive and negative energy pairs.

where the pseudospin electric $\mathcal{E}$ and magnetic $\mathcal{B}$ field in the $(n, \bar{n})$-space $\mathcal{E} = -\alpha_{gr}(\sqrt{\pi}/2)(V_n + \bar{V}_n)/2$, $\mathcal{B}_x = -\alpha_{gr}(\sqrt{\pi}/2)\tilde{V}_n$ and $\mathcal{B}_z = \sqrt{n} - \alpha_{gr}(\sqrt{\pi}/2)((V_n - \bar{V}_n)/2)$,depend on the interaction matrix elements

$$V_n = \frac{l_{\mathrm{B}}}{e^2}\sqrt{\frac{2}{\pi}}\langle n|H_{e-e}|n\rangle, \qquad \bar{V}_n = \frac{l_{\mathrm{B}}}{e^2}\sqrt{\frac{2}{\pi}}\langle \bar{n}|H_{e-e}|\bar{n}\rangle, \qquad \tilde{V}_n = \frac{l_{\mathrm{B}}}{e^2}\sqrt{\frac{2}{\pi}}\langle n|H_{e-e}|\bar{n}\rangle,$$

$$(18)$$

$\alpha_{gr} = e^2/(\hbar v_F)$ is graphene's coupling constant.

3. Results and Discussions

We must now address the regularization procedures that are necessary to extract useful predictive results from these Hartree-Fock calculations. The exchange energies V_n and $\bar{V}_n$ in Eq.(18) both diverge with cutoff M like $\sqrt{M}$ while $\mathcal{B}_z$ diverges like $\ln M$ and $\mathcal{B}_x$ goes to zero like $1/\sqrt{M}$. These large exchange energies are indeed physical because graphene's π-electron system has a high density of electrons, close to one per honeycomb lattice unit cell. This large energy is however neither easily measureable or of any great interest. Instead we want to use our Hartree-Fock theory to calculate the spacing of energy levels near the Dirac point and their dependences on the total Landau level filling factor. Progress can be made by simply choosing a convenient zero of energy, as we do in the zero-field case. We propose using the energy of the $n = 0$ Landau level, $\langle 0|H_{e-e}|0\rangle$ *evaluated for a neutral graphene sheet* as the zero of energy. In zero field the analogous choice solves all problems, but that is not true in the massless Dirac model case as we now discuss.

In order to explain the problem which remains and our resolution of this problem we go to a more microscopic level by considering properties not of the massless Dirac model but of the one-band nearest neighbour tight-binding model for graphene's π-orbitals. This model has the particle-hole symmetry property that when the Hamiltonian acts on a wavefunction which is restricted to one sublattice of the bipartite honeycomb lattice, it produces a wavefunction confined to the other sublattice. From this property it readily follows that eigenstates of the band Hamiltonian occur in positive and negative energy pairs which have opposite intersublattice phases and, importantly for the Hatree-Fock calculations, that the density-matrix of a neutral graphene sheet is just half of the trivial density matrix of a state in which all π-orbital states are full,

$$\Delta_{i',i}^{neutral} = \frac{1}{2} \, \delta_{i',i'}.$$ (19)

This property is preserved in a magnetic field and implies that the role of generalized Hubbard model interactions at the neutrality point in Hartree-Fock theory is simply to shift all energy levels by an irrelevant constant. This property is independent of the dependence of the interaction on site-separation. When translated to the continuum model, this property implies that for the case of a neutral graphene sheet both $\mathcal{E}$ in Eq.(17) should be independent of n and equal to $\langle 0|H_{e-e}|0\rangle$ and that $\mathcal{B}_x$ should vanish. Although the regularization procedure discussed above recovers this result with errors that vanish with cutoff like $1/\sqrt{M}$, the particle-hole symmetry property is so essential to the observed properties of graphene sheets that these errors are uncomfortably large at practical values of M. We therefore propose the following regularization procedure for Hartree-Fock Landau level calculations for the massless Dirac model of graphene: i) Solve the Hartree-Fock equations for neutral graphene by setting $\Delta_{0,0} = 1/2$, and $\Delta_{n,n} = (1 - sgn(n))/2$ for $n \neq 0$. ii) For the neutral case choose $\langle 0|H_{e-e}|0\rangle$ as the zero of energy and set $\mathcal{E}$ and $\mathcal{B}_x$ to zero to compensate for the violation of particle-hole symmetry caused by a finite M cut-off iii) In the case of charged graphene sheets $\Delta_{n',n}$ must be determined by a self consistent calculation in which $\mathcal{E}$ and $\mathcal{B}_x$ are replaced by the the difference between their neutral and charged system values. The Hartree-Fock energy levels of a neutral graphene sheet obtained by following i) are illustrated in Fig.(3). The logarithmic dependence of all levels on cut-off M in this figure is expected to appear experimentally as a weak logarithmic correction to the $\sqrt{B}$ dependence of Landau level energies on field expected for non-interacting electrons.

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